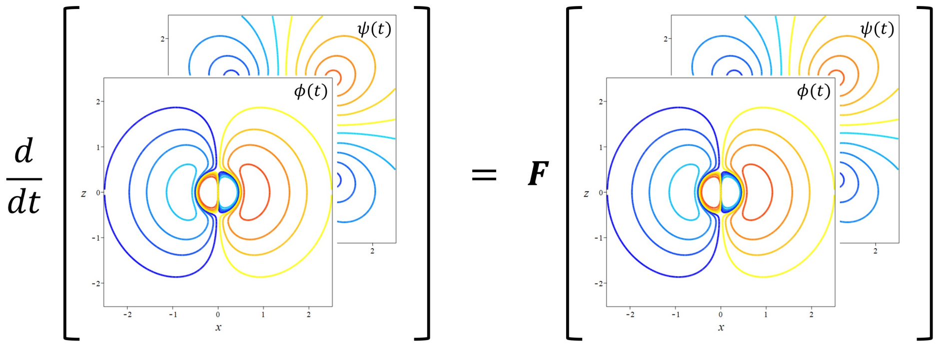
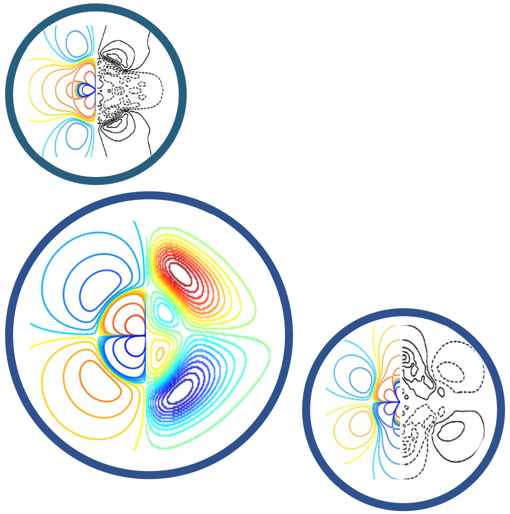


Hybrid-twin synthesis



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Overview

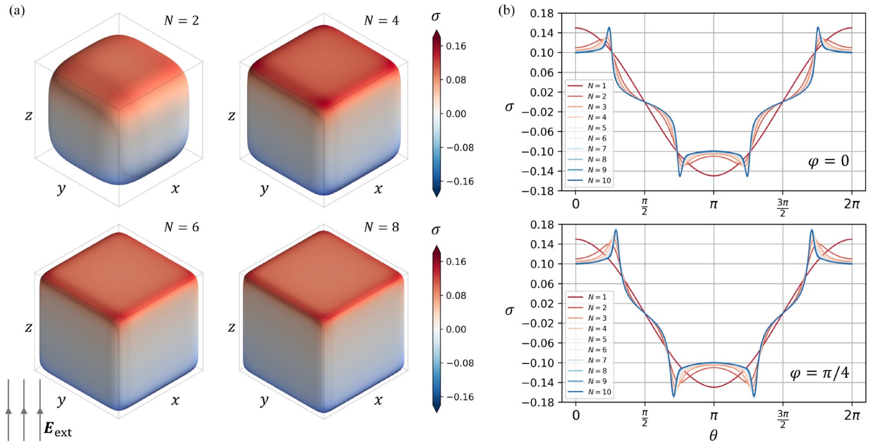
Hybrid-twin in our narrow point of view

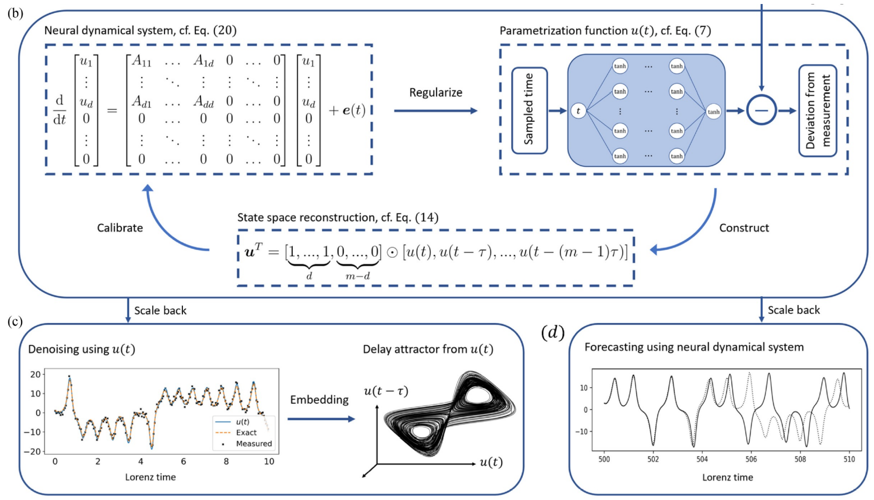
Hybrid-twin = physics + neural networks

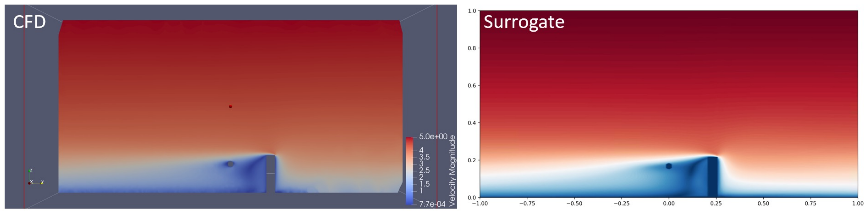
- Physics: governing equations, boundary conditions, symmetries and other equality and/or inequality constraints.
- Neural networks: nonlinear, deterministic, continuous, differentiable functions that map given input to desired outputs.
- +: the physics can be incorporated as an ansatz or as loss functions.

Problem classification

- Physics is completely known. convert initial-boundary value problems of differential equations into a minimization of loss function.
- Physics is completely unknown: identify hidden governing equations from incomplete/noisy data.
- Physics is partly known: calibrate a surrogate model for fast simulation.







Case 1: Dielectric quasi-cube in a uniform electric field

Physics

The electric potential ϕ is governed by Laplace equation

$$\nabla^2\phi = 0.$$

subjected to Dirichlet boundary conditions at origin and infinity

$$\phi_0 = -E_{\text{ext}} r\cos(\theta), \quad \text{as} \quad r\to\infty,$$

$$\phi_1 = 0, \quad \text{at} \quad r = 0,$$

and Neuman boundary condition

$$\phi_0 = \phi_1,$$

$$\nabla\phi_0\cdot\hat{\boldsymbol{n}} = \epsilon_r\nabla\phi_1\cdot\hat{\boldsymbol{n}}.$$

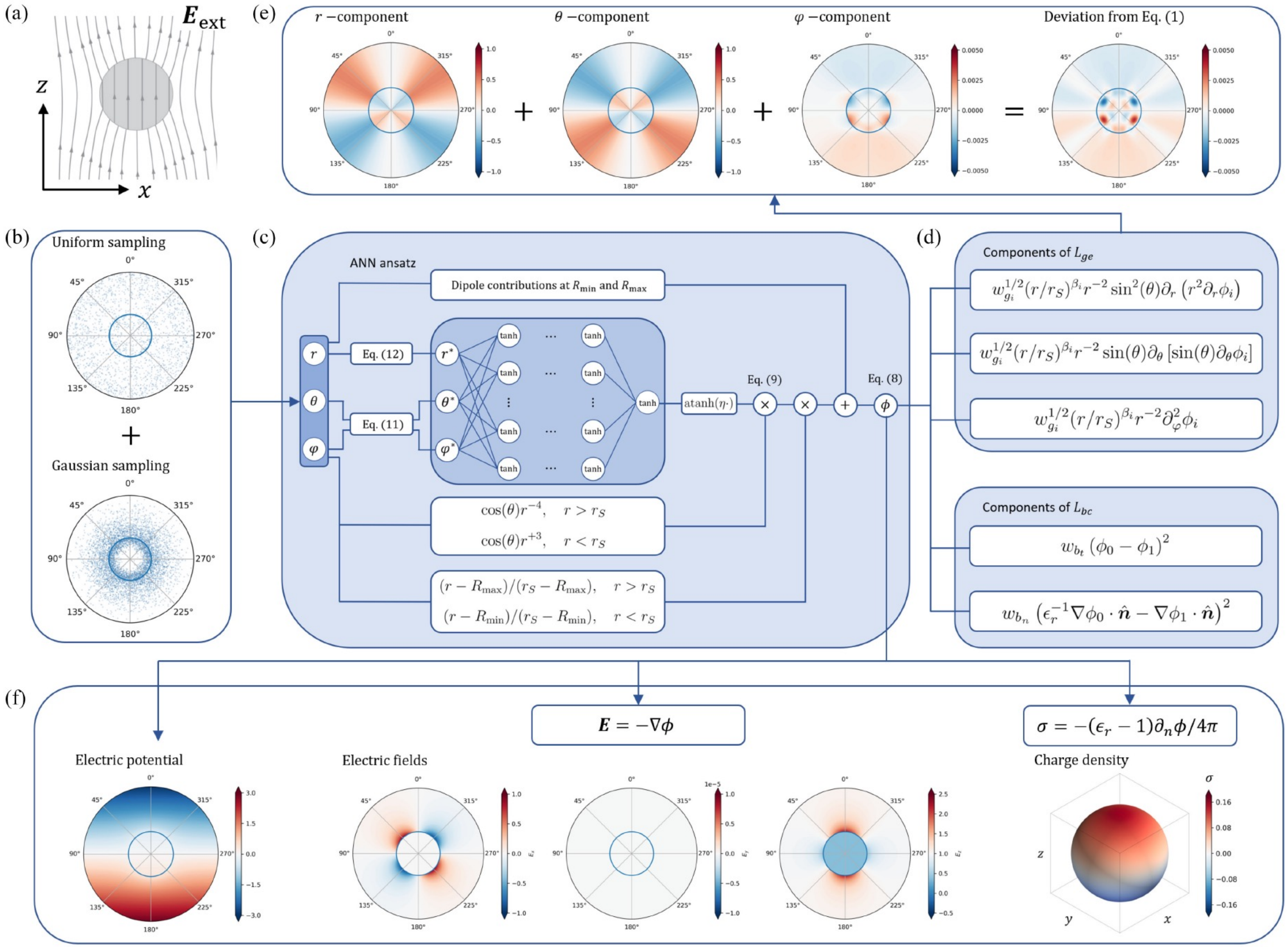
The geometry implies the following symmetries for

$$\phi(r,\theta,\varphi) = -\phi(r,\pi-\theta,\varphi),$$

$$\phi(r,\theta,\varphi) = \phi(r,\theta,-\varphi),$$

$$\phi(r,\theta,\varphi) = \phi(r,\theta,\pi+\varphi),$$

$$\phi(r,\theta,\varphi) = \phi(r,\theta,\pi-\varphi).$$



Case 2: Learning hidden neural dynamical system from noisy time series

Physics

- Time series is a function of time
- Deterministic time series is a projection of solution trajectories of a state vector onto the real axis.

Objective: recover from a noisy, incomplete observation of time series the underlying dynamical system that generates the time series.

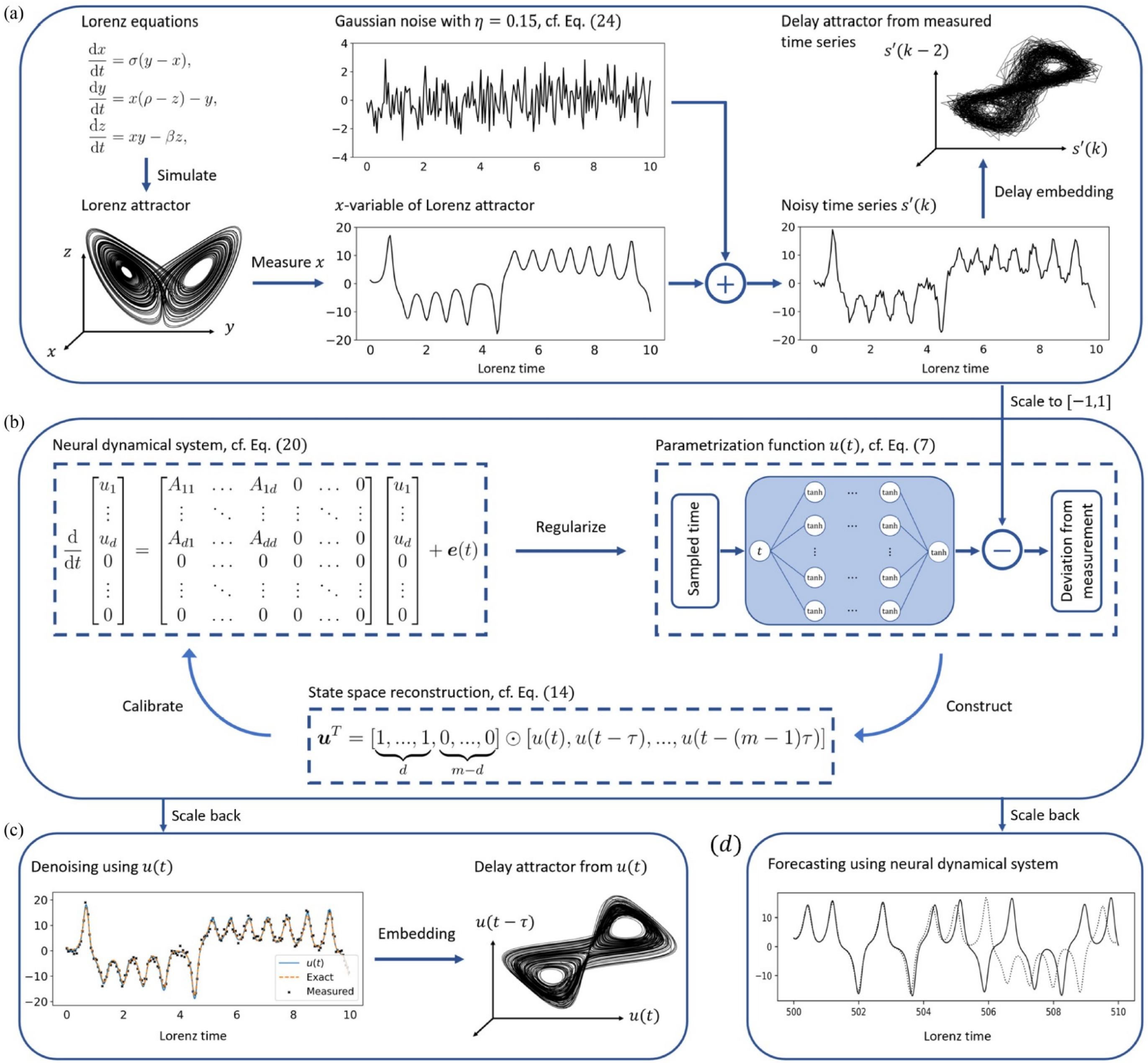
Our approach

- Since time series is a function of time

$$L_{\text{fit}} = \frac{1}{N\sigma_s^2} \sum_{k=1}^{N} [s(k) - \mathcal{N}_u(t_k; \boldsymbol{\theta}_u)]^2 ,$$

- Assuming that the time series is generated by an unknown dynamical system

$$\frac{\mathrm{d}\boldsymbol{u}(t)}{\mathrm{d}t} = \boldsymbol{A}\boldsymbol{u}(t) + \boldsymbol{e}(t) \quad \text{with} \quad \boldsymbol{A} \in \mathbb{R}^{m\times m},$$



Case 3: Surrogate model for urban wind field

Objectives

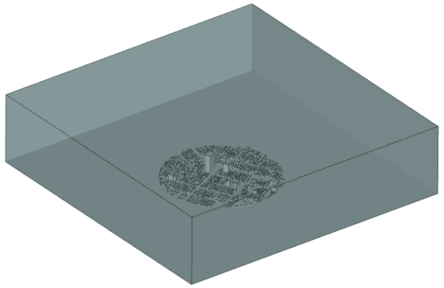
For wind field in urban environment, we aim to provide a swift and precise

1. Filtering of measurement from sensors
2. Assimilation of filtered data with the physics equations
3. Forecasting and simulation.

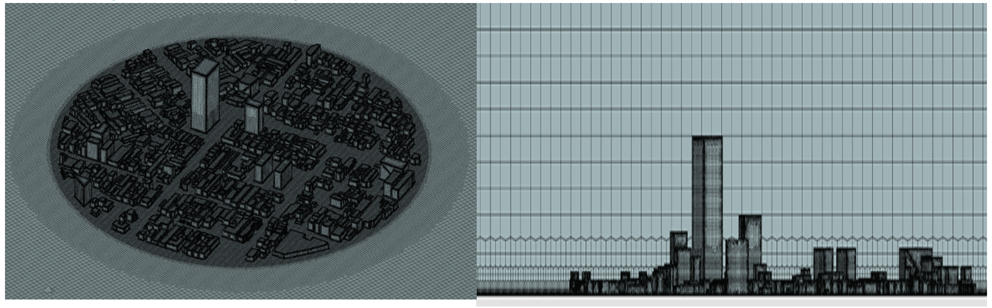
Challenges (from our point view)

Mesh & boundary conditions: -> **mesh-free/data-driven**

Far-field/meteorological

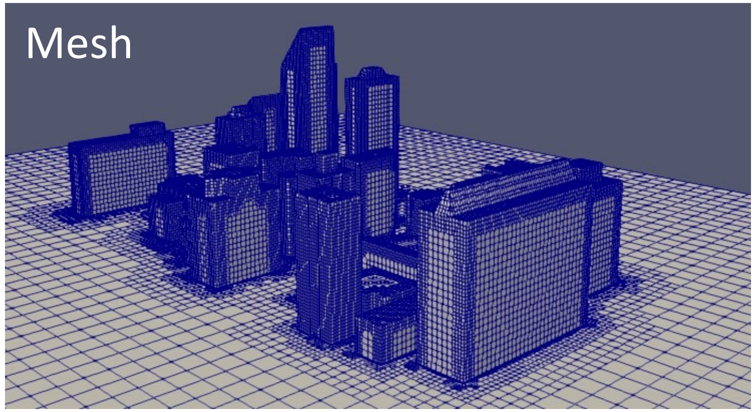


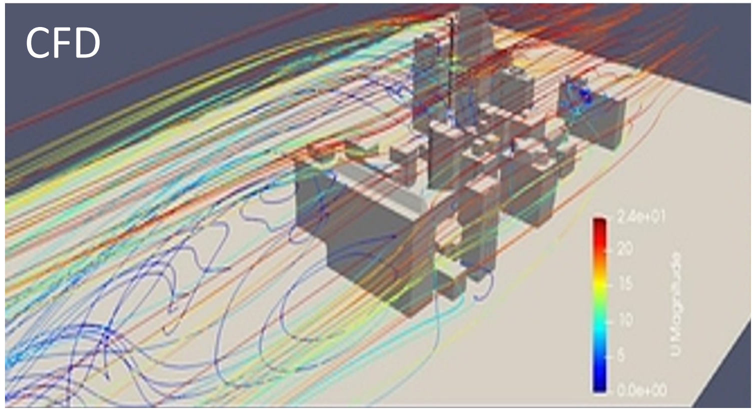
No-slip boundary condition on the walls



Governing equations: -> **surrogate model**

Numerical difficulties associated with the Navier-Stokes equations.





Navier-Stokes equations in urban environment

Navier-Stokes equations

Momentum

$$\partial_t u_x + \boldsymbol{u} \cdot \nabla u_x = -\rho^{-1} \partial_x p + \nu \nabla^2 u_x,$$
$$\partial_t u_y + \boldsymbol{u} \cdot \nabla u_y = -\rho^{-1} \partial_y p + \nu \nabla^2 u_y,$$
$$\partial_t u_z + \boldsymbol{u} \cdot \nabla u_z = -\rho^{-1} \partial_z p + \nu \nabla^2 u_z,$$

Continuity

$$\nabla \cdot \boldsymbol{u} = 0.$$

Physical boundary conditions:

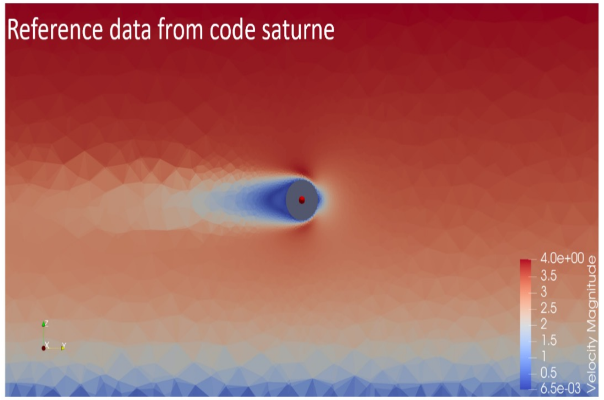
1. Canopy: meteorology
2. Border: zero velocity gradient
3. Walls: zero velocity

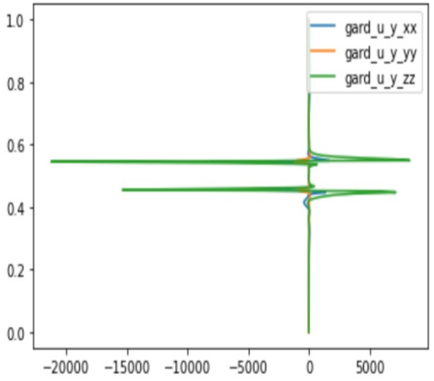
Remark on practicality

The kinematic eddy viscosity of the air

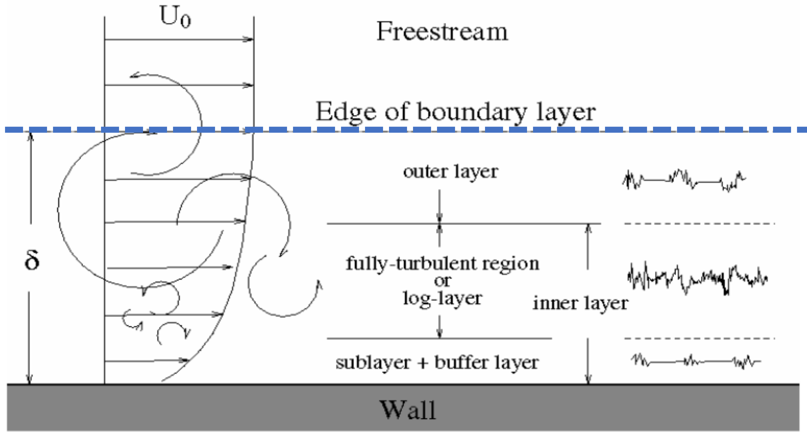
$$\nu \sim 10^{-5}$$

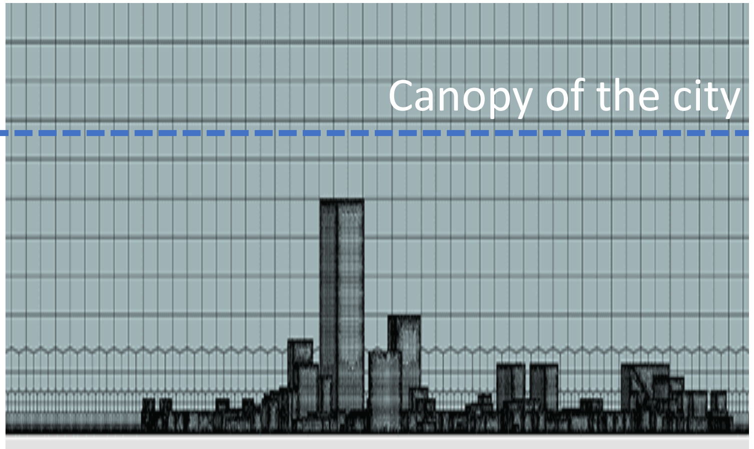
Yet the viscous term is not negligible.





Meteorological data





Comments:

1. The implementation of physical boundary conditions requires the wind field to reach a steady state, leading to a large size of the computation domain.
2. Urban wind field can be viewed as a superposition of an analytical vertical profile, where the freestream velocity is given by the meteorology, and a perturbation.

Reynolds averaged Navier-Stokes equations in urban environment

Reynolds decomposition: decompose the velocity and the pressure into a mean flow $(\boldsymbol{U}, P)$, a turbulent fluctuation $(\boldsymbol{u}', p')$, and a deviation $(\tilde{\boldsymbol{u}}, \tilde{p})$. Performing long time average

$$\tilde{\boldsymbol{u}} = \overline{\boldsymbol{u} - \boldsymbol{U}} = \overline{\boldsymbol{u}} - \boldsymbol{U}, \quad \tilde{p} = \overline{p - P} = \overline{p} - P,$$

And evoking the turbulent-viscosity hypothesis

$$-\overline{u_i' u_j'} + \frac{1}{3}\delta_{ij}\overline{u_i' u_i'} = \nu_t \left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} \right),$$

we obtain

$$\overline{u}_x \partial_x \overline{u}_x + \overline{u}_y \partial_y \overline{u}_x + \overline{u}_z \partial_z \overline{u}_x = -\rho^{-1} \partial_x \overline{p}_\Sigma + \frac{\partial \nu_\Sigma}{\partial x_j} \left(\frac{\partial \overline{u}_x}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x} \right) + \nu_\Sigma \nabla^2 \overline{u}_x,$$

$$\overline{u}_x \partial_x \overline{u}_y + \overline{u}_y \partial_y \overline{u}_y + \overline{u}_z \partial_z \overline{u}_y = -\rho^{-1} \partial_y \overline{p}_\Sigma + \frac{\partial \nu_\Sigma}{\partial x_j} \left(\frac{\partial \overline{u}_y}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial y} \right) + \nu_\Sigma \nabla^2 \overline{u}_y,$$

$$\overline{u}_x \partial_x \overline{u}_z + \overline{u}_y \partial_y \overline{u}_z + \overline{u}_z \partial_z \overline{u}_z = -\rho^{-1} \partial_z \overline{p}_\Sigma + \frac{\partial \nu_\Sigma}{\partial x_j} \left(\frac{\partial \overline{u}_z}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial z} \right) + \nu_\Sigma \nabla^2 \overline{u}_z,$$

Remark: the presence of turbulence augments the mean pressure field with turbulent kinetic energy and augments the molecular kinematic viscosity with eddy viscosity

$$\overline{p}_\Sigma = \overline{p} + \frac{1}{3}\rho\overline{u_i' u_i'} \quad \text{and} \quad \nu_\Sigma(x,y,z) = \nu + \nu_t(x,y,z).$$

A priori knowledge

1. Velocity $\overline{\boldsymbol{u}}$ vanishes inside the buildings

$$\text{mask}(x,y,z) = \begin{cases} 1, & \text{if} \quad (x,y,z) \in \Omega_i, \\ 0, & \text{if} \quad (x,y,z) \in \partial\Omega_b, \\ 0, & \text{if} \quad (x,y,z) \in \Omega_b, \end{cases}$$

Remark: classification with binary cross entropy loss.

2. In the absence of budlings, the mean velocity

$$U_x(z) = U\cos(\varphi)\frac{\ln(z/z_0+1)}{\ln(Z/z_0+1)}, \quad U_y(z) = U\sin(\varphi)\frac{\ln(z/z_0+1)}{\ln(Z/z_0+1)},$$

Which also implies that the deviation vanishes on the ground and at the canopy of the city

$$g(z) = \sin\left(\frac{h\pi z}{L_z}\right),$$

3. To be compatible with the logarithmic wind profile, the eddy viscosity is linear

$$\nu_t(z) = \frac{u_\tau^2}{\partial_z \sqrt{U_x^2 + U_y^2}} = \frac{\kappa^2 U(z+z_0)}{\ln(Z/z_0+1)},$$

Hybrid twin synthesis

Physics are intertwined with neural networks via neural ansatz and loss functions.

Neural ansatz

$$\overline{\boldsymbol{u}}_\theta(x,y,z,\varphi) = \mathrm{mask}(x,y,z)\left[\boldsymbol{U}(z) + gU\cdot\mathcal{N}_u(x,y,z,\varphi;\boldsymbol{\theta}_{\tilde{u}})\right],$$

$$p_\theta(x,y,z,\varphi) = \mathrm{mask}(x,y,z)\mathcal{N}_p(x,y,z,\varphi;\boldsymbol{\theta}_p)$$

$$\nu_\theta(x,y,z,\varphi) = \frac{\kappa^2 U(z+z_0)}{\ln(Z/z_0+1)}\mathcal{N}_\nu(x,y,z,\varphi;\boldsymbol{\theta}_\nu),$$

such that the asymptotic behavior, the no-slip boundary conditions are satisfied by construction, leaving (i) RANS model; and (ii) incompressibility constraints to be imposed.

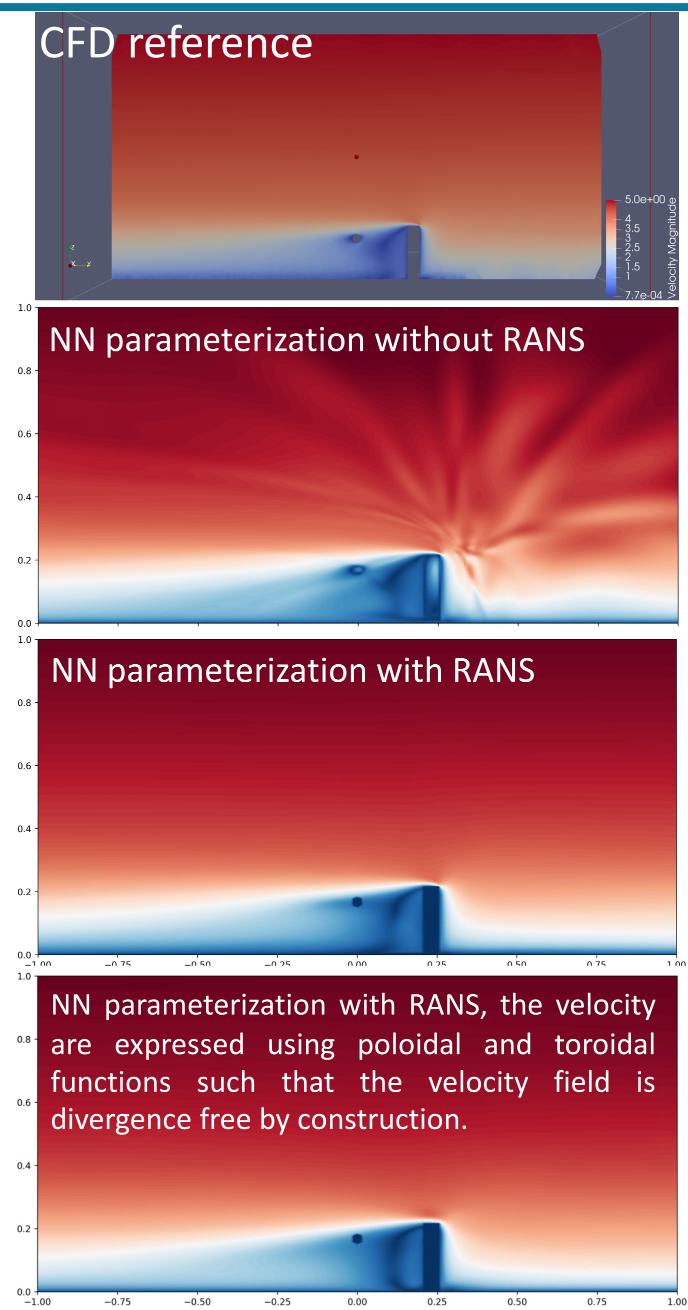
Remark: the incompressibility constraints can be incorporated into the neural ansatz through poloidal-toroidal decomposition

$$\tilde{\boldsymbol{u}}^* = \nabla^* \times \psi^*(x,y,z)\hat{\boldsymbol{z}} + \nabla^* \times \nabla^* \times \phi^*(x,y,z)\hat{\boldsymbol{z}},$$

Loss functions our loss functions consist of

(i) deviation of the approximated velocity, pressure, and eddy viscosity to reference data; and

(ii) the residue of the incompressibility constraints and RANS model.

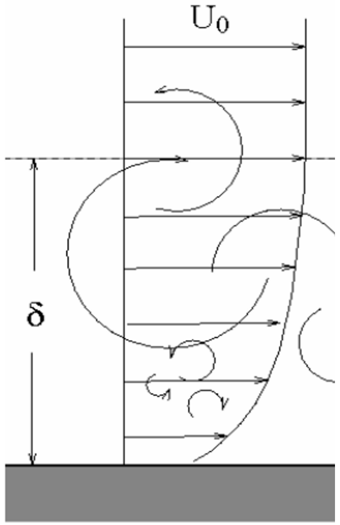


Surrogate model (demo)

Problem setup

We consider the flow past a cylinder and a sphere, the boundary condition in the far-field is given by a logarithmic wind profile characterized by the magnitude U_0 and the orientation φ_0 of the wind. Given the symmetry of the geometries, we run 8 independent simulation with fixed U_0 and various values of $\varphi_0 \in [90, 270]$ degrees. We reserve the case $\varphi_0 = 135$ degrees as our testing dataset.

Objective: To obtain a surrogate model that generates the desired wind field for any given values of (U_0, φ_0).




```
Number of meshpoints on buildings (surface): 8744
Number of meshpoints in buildings (volume): 25138
Number of meshpoints in atmoshphere: 79432
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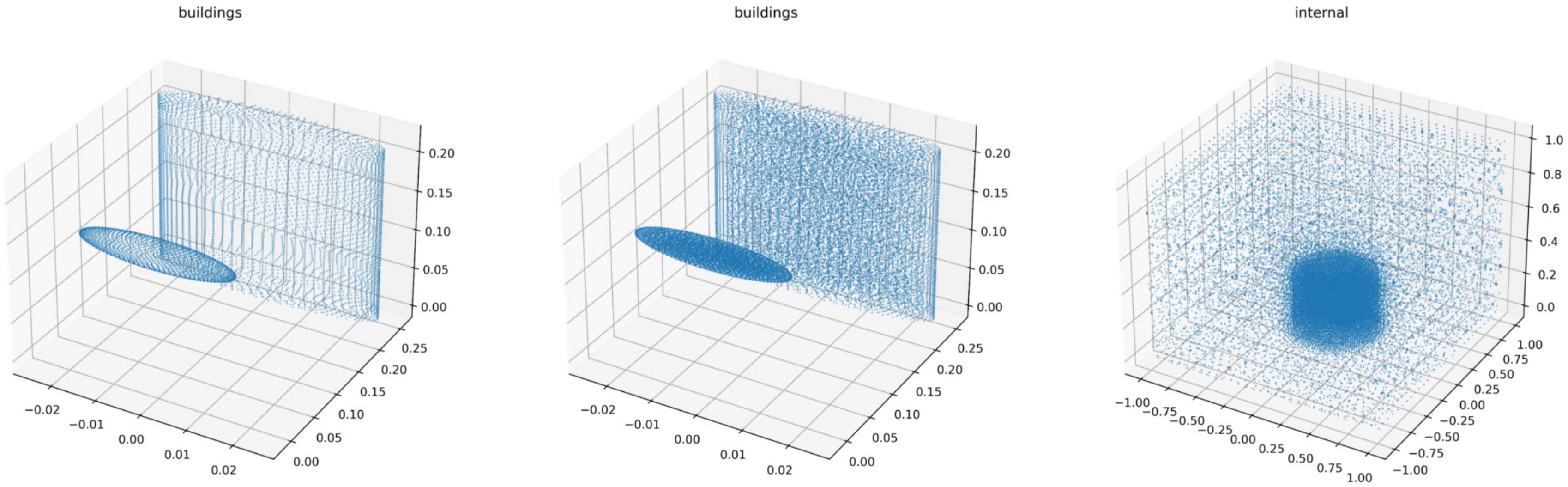

Conclusions

- Physics can be incorporated into neural networks through (i) ansatz; and (ii) loss functions.
- By exploiting self-consistency, we can (i) recover hidden physics from data; and (ii) bring regularization to the measured data.
- However, the use of neural networks do not mitigate numerical challenges originated from the governing equations.
- Minimizing loss functions involving differential equations using first order gradient descent method may not be optimal, especially when singularity developed in the simulation domain.
- When there are multiple loss functions originated from different constraints, balancing multiple loss functions can be challenging.